High-resolution 2D MR spectroscopy via intermolecular multiple-quantum coherences

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Introduction

Intermolecular multiple-quantum coherences (iMQCs) have been utilized to achieve high-resolution 1D spectrum under inhomogeneous fields[1]. The high-resolution iMQC spectroscopy uses two-dimensional approach to average out inhomogeneous broadenings by correlating the iMQC transition and the conventional single-quantum coherence (SQC) one. After the shearing processes, the high-resolution 1D spectrum free of line broadening can be extracted from the projection along one dimension of the processed 2D spectrum; the information along the other dimension, however, will be discarded since it contains only inhomogeneous broadenings. The high-resolution iMQC spectroscopy have been applied to the MRS of the field-distorted voxel, where the spectral linewidths are broadened by the magnetic field gradients caused by susceptibility differences between tissues, bones and air[2].

2D MRS such as *J*-resolved spectroscopy (J-RES) and COSY have been explored to obtain better signal separations in the 2D spectra[3]. However, line broadenings still occur in these 2D spectra and lead to overlapping of adjacent resonances. In this abstract, we extend the 1D high-resolution iMQC spectroscopy to 2D, using a three-dimensional approach to achieve a 2D MRS free of inhomogeneous broadening.

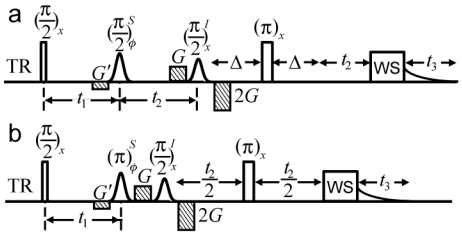

Fig. 1. High-resolution MRS sequences via 3D iMQCs: (a) COSY and (b) J-RES.

Methods

Similar to 1D high-resolution spectroscopy via two-dimensional iMQCs, the directly-acquired dimension (t_3) of the proposed three dimensional approach is conventional SQCs and is subject to inhomogeneous broadenings. On the other hand, the other two dimensions (t_1 and t_2) are either refocused iMQCs or spin echoes, both of which are insensitive to inhomogeneous fields. Normally, the acquisition time of the 3D spectrum would be unbearable for *in vivo* measurements. Therefore, fast acquisition schemes such as delay acquisition and foldover correction (FOC)[4], can be used to reduce one of the indirect spectral width, and thus the scanning time.

The sequences of high-resolution COSY and J-RES are presented in Fig. 1a and 1b, respectively. In the COSY sequence, the t_1 and t_2 periods are iZQC and iDQC evolutions, respectively. The t_2 period utilizes the delay-acquisition scheme to reduce the scanning time, thus the apparent *J* coupling constant is scaled up by 3 times. In the J-RES sequence, the t_1 period is iZQCs and the t_2 period is spin echo. The t_1 period utilizes the FOC scheme to speed up the scanning.

All experiments were performed using a Varian NMR System 11.7 T with a 5 mm indirect detection probe. The parameters of coherence selective gradients are $G' = 0.07$ T m^{-1} $\times 1.2$ ms and $G = 0.16$ T m^{-1} $\times 1.2$ ms respectively. A 2-step phase cycling was applied: $\phi = (x, y)$ and receiver $= (x, -x)$. A solution of butanone in cyclohexane (molar ratio = 1:1000) was for the COSY measurements. $192 \times 16 \times 300$ points were acquired with spectral widths of $1200 \times 100 \times 1200$ Hz (F1 $\times$ F2 $\times$ F3) in 2 h. TR / TE = 1 / 0.1 s . A water solution containing 10 mM histidine and 10 mM lactate was used for the J-RES experiments. $12 \times 10 \times 256$ points were acquired with spectral widths of $100 \times 40 \times 4000$ Hz (F1 $\times$ F2 $\times$ F3) in 20 min. The average number was 4 and TR = 2 s.

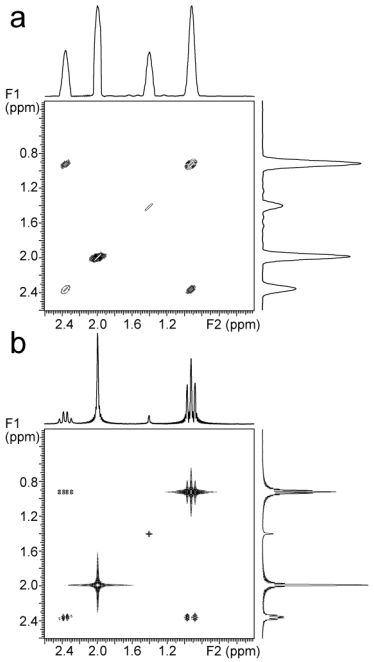

Fig. 2. (a) Conventional COSY and (b) high resolution COSY via 3D iMQCs.

Results and discussion

A conventional COSY spectrum is presented in Fig. 2a. Broadened lines stretch at the diagonal direction. The projections of both dimensions are subject to line broadenings. The high-resolution COSY spectrum is presented in Fig. 2b. Both dimensions are free of line broadening. The *J* coupling constants in the F2 dimension are scaled up by 3 times. The conventional and high-resolution J-RES spectra are presented in Fig. 3a and 3b, respectively. The broadened lines stretch along the F2 dimension in Fig. 3a and cause overlapping of strongly-coupled resonances of histidine. In Fig. 3b, these two resonances are well separated and the strongly-coupled artifact can be observed.

The above results primarily present the feasibility of the proposed 2D MRS sequences. For the SNR consideration, the iMQC based high-resolution sequences are more applicable on animal studies with high-field scanning systems. The scanning time of the 3D sequences can be further reduced by using multi-acquisition scheme proposed by Warren's group[5]. Further *in vivo* experiments are under work.

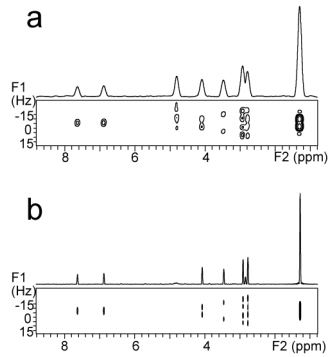

Fig. 3. (a) Conventional J-RES spectrum and (b) high resolution J-RES spectrum via 3D iMQCs.

Acknowledgments

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Reference

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